

Page 1

Berch
10/694619

=> dis his

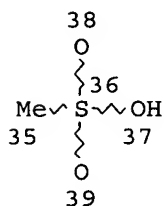
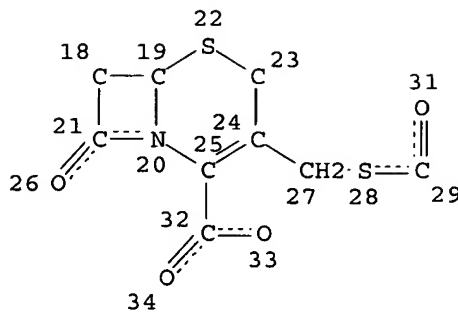
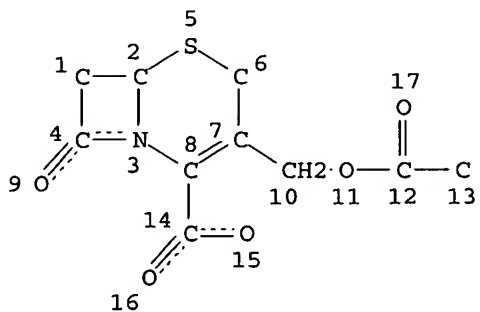
(FILE 'HOME' ENTERED AT 14:13:43 ON 13 DEC 2005)

FILE 'CASREACT' ENTERED AT 14:13:57 ON 13 DEC 2005

L1 STR
L2 2 S L1
L3 STR L1
L4 1 S L3
L5 1 S L3 FUL

=> d l5 que stat;d fhit bib abs

L3 STR



2-sided

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 38

STEREO ATTRIBUTES: NONE

L5 1 SEA FILE=CASREACT SSS FUL L3 (1 REACTIONS)

100.0% DONE 16 VERIFIED

1 HIT RXNS

1 DOCS

SEARCH TIME: 00.00.01

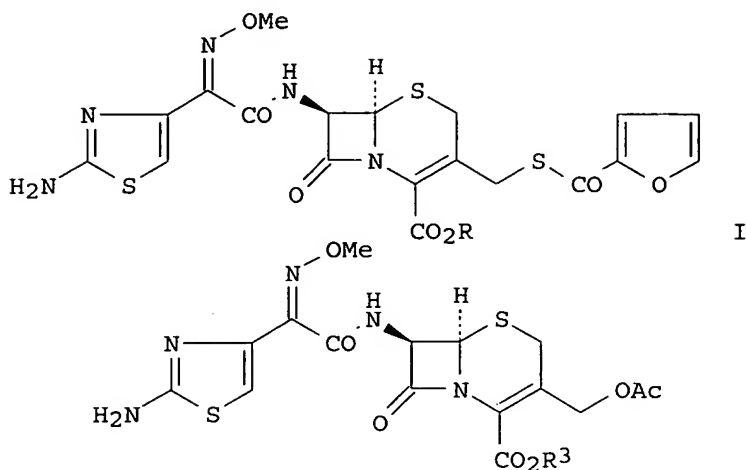
L5 ANSWER 1 OF 1 CASREACT COPYRIGHT 2005 ACS on STN

RX(1) OF 1 A + B ==> C

Prepared by: Mary Hale @2-2507 Rem Bldg 1D86

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 2004132996	A1	20040708	US 2003-694619	20031027
PRAI	IN 2002-MU938		20021029		
OS	MARPAT 141:88965				
GI					

↑
This work



AB A process for preparation of ceftiofur sodium I (R = Na) possessing high stability and having purity of more than 97% and substantially free of impurities, was disclosed. The process comprised reacting cefotaxime or its derivative II (R₃ = H, alkali metal, alkaline earth metal, group forming an easily hydrolyzable ester) with 2-thiofuroic acid, employed in a molar proportion of 1.5 to 3.0 mol per mol of II, in the presence of acetonitrile as solvent and in the presence of large excess of methanesulfonic acid, employed in molar proportions of 12 to 18 mol per mol of II, and at a temperature of between -5° C. to 30° C. to give after necessary neutralization of the alkali or alkaline earth metal or removal of the ester group of the 4-carboxylic acid function, wherever applicable, ceftiofur I (R = H), possessing high stability and having purity of more than 97% and substantially free of impurities. Further, converting the ceftiofur to its salt with an organic amine by treating a solution of ceftiofur in a mixture of water and a water-miscible organic solvent with an organic amine, at a temperature ranging from -10° C. to 10° C., reacting of the amine salt thus obtained with a sodium metal carrier in a mixture of water and water-miscible organic solvent and in presence of sodium hydrogen sulfite to give the desired I (R = Na).

=> => dis his

(FILE 'HOME' ENTERED AT 14:13:43 ON 13 DEC 2005)

FILE 'CASREACT' ENTERED AT 14:13:57 ON 13 DEC 2005

L1 STR
L2 2 S L1
L3 STR L1
L4 1 S L3

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COST IN U.S. DOLLARS          SINCE FILE      TOTAL
                               ENTRY      SESSION
FULL ESTIMATED COST          242.07      242.28

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)  SINCE FILE      TOTAL
                                               ENTRY      SESSION
CA SUBSCRIBER PRICE          -0.68      -0.68
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FILE 'REGISTRY' ENTERED AT 14:22:59 ON 13 DEC 2005
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Property values tagged with IC are from the ZIC/VINITI data file
 provided by InfoChem.

STRUCTURE FILE UPDATES: 12 DEC 2005 HIGHEST RN 869770-56-9
 DICTIONARY FILE UPDATES: 12 DEC 2005 HIGHEST RN 869770-56-9

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

Please note that search-term pricing does apply when
 conducting SmartSELECT searches.

```
*****
*
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
*
*****
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Structure search iteration limits have been increased. See HELP SLIMITS
 for details.

REGISTRY includes numerically searchable data for experimental and
 predicted properties as well as tags indicating availability of
 experimental property data in the original document. For information
 on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

=> => dis his l16-;d l16 que stat;d l17 que stat;fil caplus;s (l19 or l20) and l17

(FILE 'REGISTRY' ENTERED AT 14:22:59 ON 13 DEC 2005)

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L17      469 S L14 FUL
L18      11557 S L16 OR L16
L19      2558 S L18 RAN=(,55371-13-6)
L20      9000 S L18 RAN=(55371-13-6,)
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L10 STR

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	ENTRY	SESSION
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DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-0.68

FILE 'CAPLUS' ENTERED AT 14:25:12 ON 13 DEC 2005
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FILE COVERS 1907 - 13 Dec 2005 VOL 143 ISS 25
 FILE LAST UPDATED: 12 Dec 2005 (20051212/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

<http://www.cas.org/infopolicy.html>

8924 L19
 7754 L20
 500 L17
 L21 242 (L19 OR L20) AND L17

=> => dis his l24-;fil caplus

(FILE 'REGISTRY' ENTERED AT 14:25:55 ON 13 DEC 2005)
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 L25 15649 S L24 OR L24
 L26 6650 S L25 RAN=(,129695-40-5)
 L27 9000 S L25 RAN=(129695-40-5,)

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	ENTRY	SESSION
FULL ESTIMATED COST	162.39	728.84
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	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-0.68

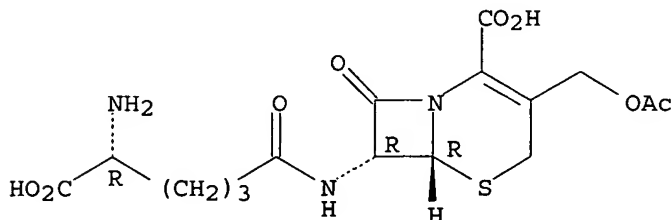
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Prepared by: Mary Hale @2-2507 Rem Bldg 1D86

nine of the most useful models for antimicrobial selection reported to date. Finally, a virtual screening of 87 new compds. reported in the anti-infective field with antibacterial activities is developed showing the ability of the models to identify new leads as antibacterial.

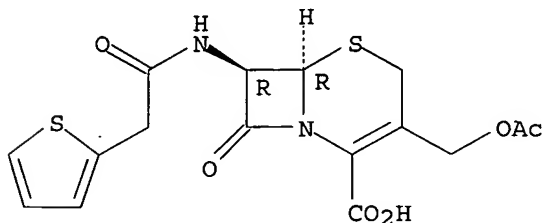
IT 61-24-5, Cephalosporin C 153-61-7, Cefalotin
 804-53-5 859-07-4, Cefaloram 886-86-2,
 Metacaine 1421-68-7, Amidefrine mesylate 3577-01-3,
 Cefaloglycin 8067-09-2, Antibiotic 810A 23239-41-0,
 Cefacetrile sodium 24356-60-3, Cefapirin sodium
 32178-82-8, 7-(5-Amino-5-carboxyvaleramido)-7-
 methoxycephalosporanic acid 33075-00-2, Cefathiamidine
 34279-77-1, Cephamycin B 36920-48-6, Cefoxazole
 39685-31-9, Cefuracetime 51159-12-7, Antibiotic BL-S217
 56083-50-2, Antibiotic C-2801X 64485-93-4, Cefotaxime
 sodium 69132-42-9, Ceftioxide 69200-65-3
 80370-57-6, Ceftiofur 82956-11-4, Futhan
 89201-82-1 852448-72-7
 RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic
 use); BIOL (Biological study); USES (Uses)
 (atom, atom-type, and total nonstochastic and stochastic quadratic
 fingerprints as promising approach for modeling antibacterial activity)
 RN 61-24-5 CAPLUS
 CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
 3-[(acetyloxy)methyl]-7-[[[(5R)-5-amino-5-carboxy-1-oxopentyl]amino]-8-oxo-
 , (6R,7R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



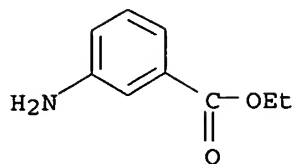
RN 153-61-7 CAPLUS
 CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
 3-[(acetyloxy)methyl]-8-oxo-7-[(2-thienylacetyl)amino]-, (6R,7R)- (9CI)
 (CA INDEX NAME)

Absolute stereochemistry.



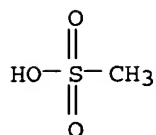
RN 804-53-5 CAPLUS
 CN 2H-Benzo[a]quinolizin-2-one, 1,3,4,6,7,11b-hexahydro-9,10-dimethoxy-3-(2-
 methylpropyl)-, (3R,11bR)-rel-, methanesulfonate (9CI) (CA INDEX NAME)

CM 1



CM 2

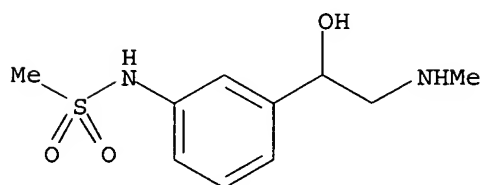
CRN 75-75-2
CMF C H4 O3 S



RN 1421-68-7 CAPLUS
CN Methanesulfonamide, N-[3-[1-hydroxy-2-(methylamino)ethyl]phenyl]-, monomethanesulfonate (salt) (9CI) (CA INDEX NAME)

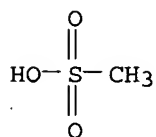
CM 1

CRN 37571-84-9
CMF C10 H16 N2 O3 S

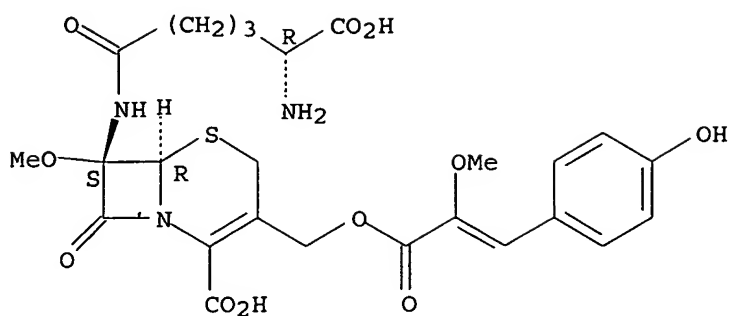


CM 2

CRN 75-75-2
CMF C H4 O3 S

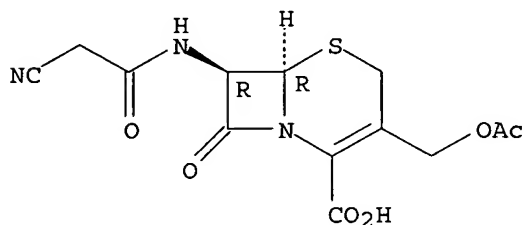


RN 3577-01-3 CAPLUS
CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 3-[(acetyloxy)methyl]-7-[[[(2R)-aminophenylacetyl]amino]-8-oxo-, (6R,7R)- (9CI) (CA INDEX NAME)



RN 23239-41-0 CAPLUS
 CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
 3-[(acetyloxy)methyl]-7-[(cyanoacetyl)amino]-8-oxo-, monosodium salt,
 (6R,7R)- (9CI) (CA INDEX NAME)

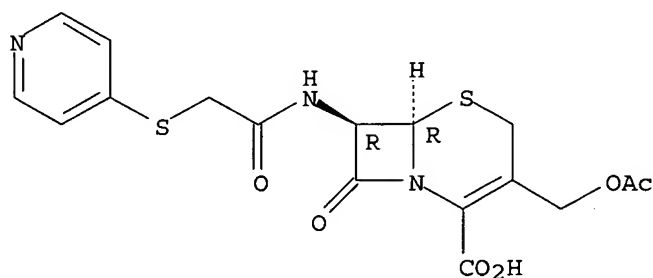
Absolute stereochemistry.



● Na

RN 24356-60-3 CAPLUS
 CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
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 monosodium salt, (6R,7R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

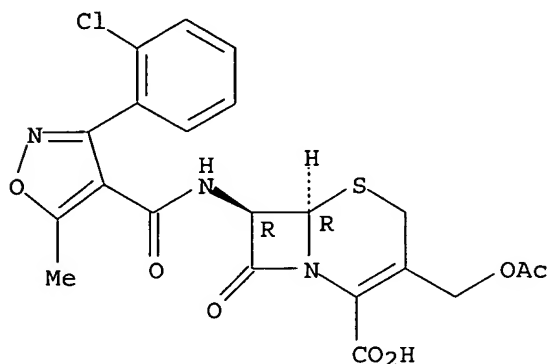


● Na

RN 32178-82-8 CAPLUS
 CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,

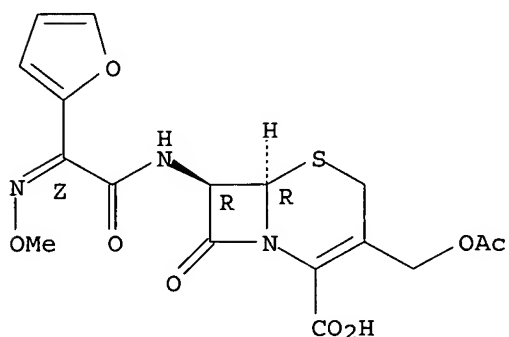
RN 36920-48-6 CAPLUS
 CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
 3-[(acetyloxy)methyl]-7-[[[3-(2-chlorophenyl)-5-methyl-4-
 isoxazolyl]carbonyl]amino]-8-oxo-, (6R,7R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



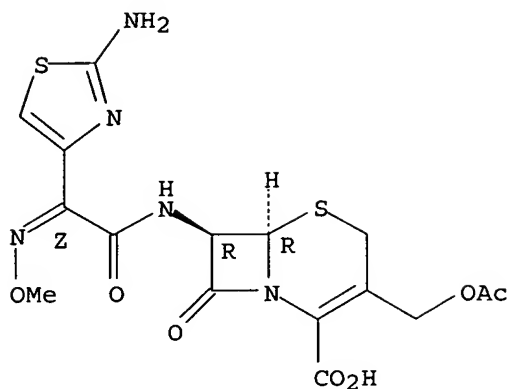
RN 39685-31-9 CAPLUS
 CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
 3-[(acetyloxy)methyl]-7-[[[(2Z)-2-furanyl(methoxyimino)acetyl]amino]-8-oxo-
 , (6R,7R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
 Double bond geometry as shown.



RN 51159-12-7 CAPLUS
 CN Pyridinium, 4-[[[2-[[[6R,7R]-3-[(acetyloxy)methyl]-2-carboxy-8-oxo-5-thia-1-
 azabicyclo[4.2.0]oct-2-en-7-yl]amino]-2-oxoethyl]thio]-1-methyl- (9CI)
 (CA INDEX NAME)

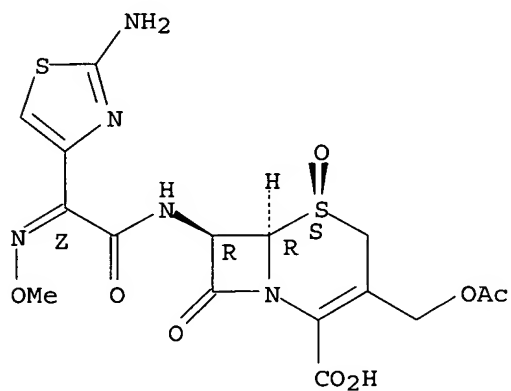
Absolute stereochemistry.



● Na

RN 69132-42-9 CAPLUS
 CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
 3-[(acetyloxy)methyl]-7-[[[(2Z)-(2-amino-4-thiazolyl)(methoxyimino)acetyl]a
 mino]-8-oxo-, 5-oxide, (5S,6R,7R)- (9CI) (CA INDEX NAME)

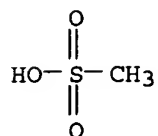
Absolute stereochemistry.
 Double bond geometry as shown.



RN 69200-65-3 CAPLUS
 CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
 7-[(5-amino-5-carboxy-1-oxopentyl)amino]-3-[[[3-(4-hydroxyphenyl)-2-
 methoxy-1-oxo-2-propenyl]oxy]methyl]-7-methoxy-8-oxo-, (6R,7S)- (9CI) (CA
 INDEX NAME)

Absolute stereochemistry.
 Double bond geometry unknown.

CRN 75-75-2
CMF C H4 O3 S

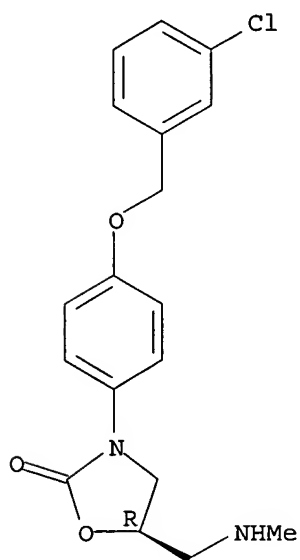


RN 89201-82-1 CAPLUS
CN 2-Oxazolidinone, 3-[4-[(3-chlorophenyl)methoxy]phenyl]-5-
[(methylamino)methyl]-, (5R)-, monomethanesulfonate (9CI) (CA INDEX NAME)

CM 1

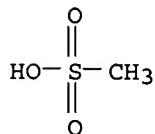
CRN 84145-89-1
CMF C18 H19 Cl N2 O3

Absolute stereochemistry.



CM 2

CRN 75-75-2
CMF C H4 O3 S

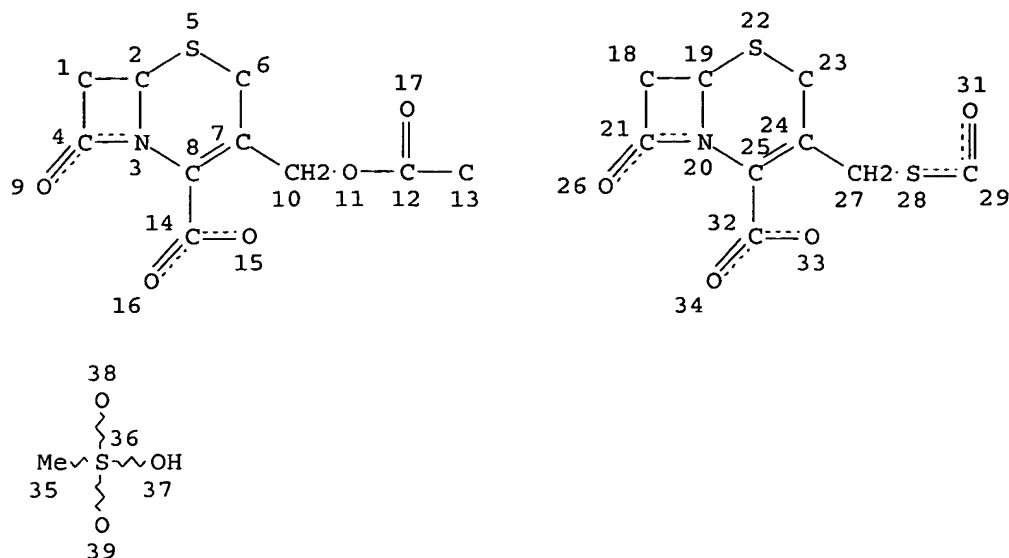


RN 852448-72-7 CAPLUS

Page 21

L28 1 S (L26 OR L27) AND L21

=> d 15 que stat;d 16 que stat;d l16 que stat;d l18 que stat;d l24 que stat
L3 STR



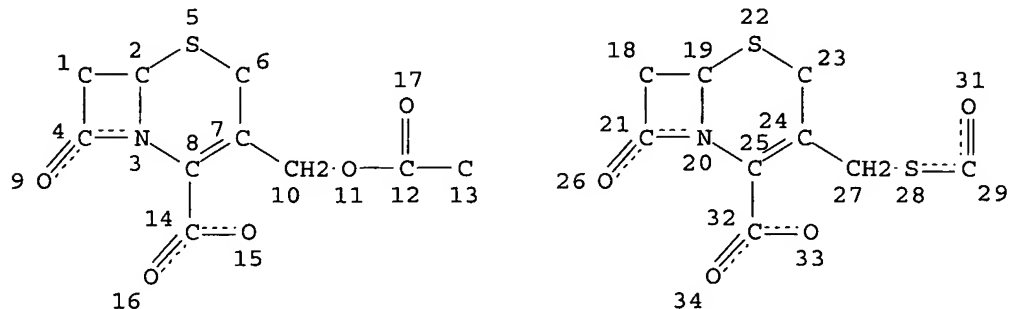
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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 38

STEREO ATTRIBUTES: NONE
L5 1 SEA FILE=CASREACT SSS FUL L3 (1 REACTIONS)

100.0% DONE 16 VERIFIED 1 HIT RXNS 1 DOCS
SEARCH TIME: 00.00.01

L1 STR



NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

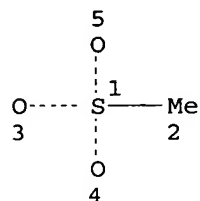
Prepared by: Mary Hale @2-2507 Rem Bldg 1D86

DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 17

STEREO ATTRIBUTES: NONE
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L18 11557 SEA FILE=REGISTRY ABB=ON PLU=ON L16 OR L16

L22 STR



NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 5

STEREO ATTRIBUTES: NONE
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100.0% PROCESSED 389720 ITERATIONS 15649 ANSWERS
SEARCH TIME: 00.00.04

=> log y		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	5.84	734.68
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-0.73	-1.41

STN INTERNATIONAL LOGOFF AT 14:29:21 ON 13 DEC 2005